Status of the transition from the legacy ENDF format to GNDS

D. Brown

National Nuclear Data Center

BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

Outline

- History
- The GNDS Project
- Code support and API
- Format Overview
- Current status: GNDS-1.9 vs. 1.10

Outline

- History
- The GNDS Project
- Code support and API
- Format Overview
- Current status: GNDS-1.9 vs. 1.10

Before the ENDF format

- **By 1960, there were many data efforts worldwide**
  - different formats
  - often hard-coded libraries
  - proprietary data
  - Notable efforts: UKNDL (AWE, UK), NDA library (US), ENDL (LRL, US)
- **~1962 H. Honeck (BNL), A. Henry (Westinghouse), G. Joanou (GA) met at Colony Restaurant in DC decided on action**
  - requested Reactor Mathematics and Computation Division of ANS sponsor 2 meetings to link databases

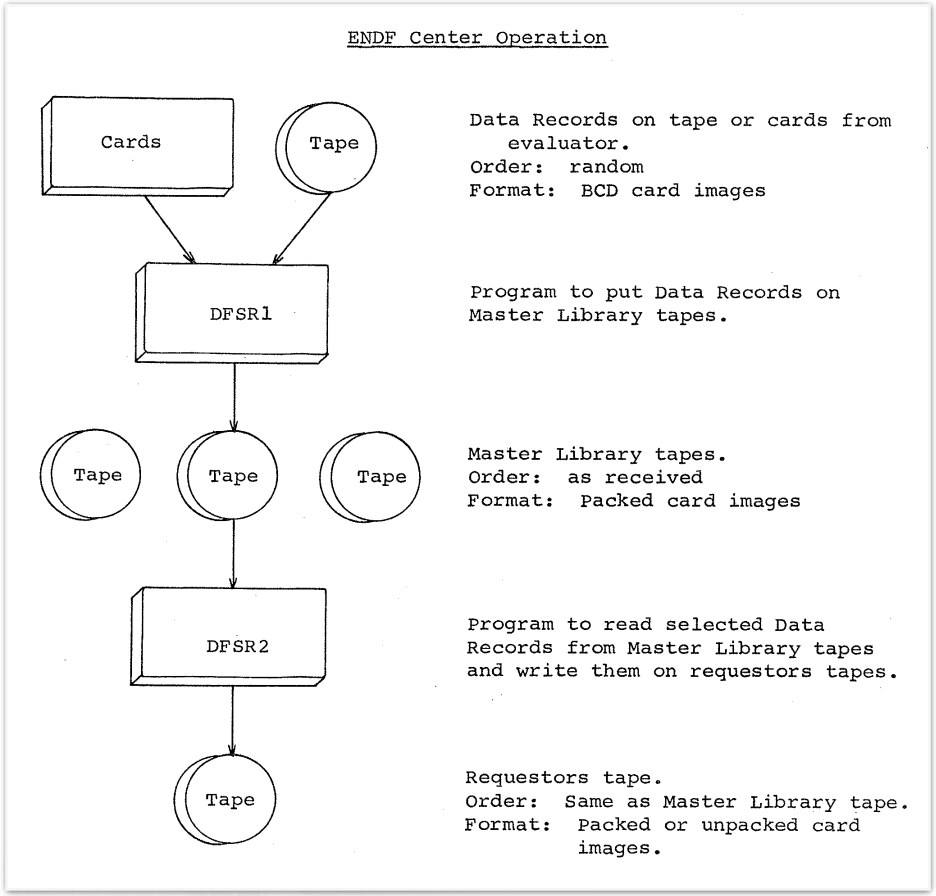
http://www.streetsofwashington.com/2013/10/fine-dining-in-washington-dc-in-1950s.html

The first ENDF formats

- **ENDF/A documented in BNL-8381, released in 1965, based on UK's UKNDL with data from other libraries**
- **ENDF/B first documented in ENDF-102 (1966)**
- **ENDF/B-I library released in July 1968**
  - Back then there was no "I", who would have predicted 50 years later we'd be releasing version "VIII.0"
- **Original data project funded by Atomic Energy Commission in US**

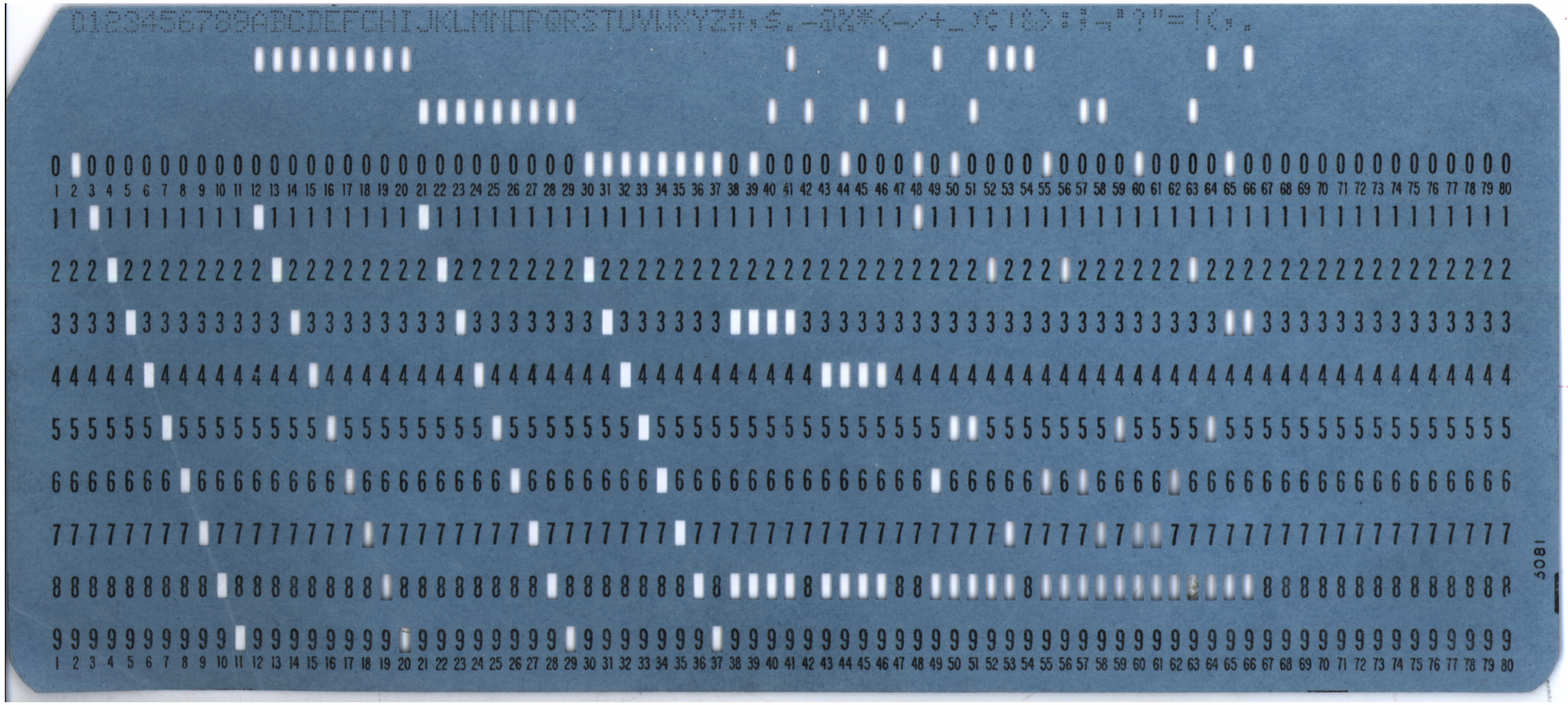
ENDF format was (and still is) tied to original infrastructure

- **Original format designed to fit on IBM 80 column punchcards**
  - Evaluations actually were occasionally submitted on punchcards
- **Original data stored on magnetic tapes**
- **It was possible to request ENDF data on tapes and/or punchcards**
  - Punchcard format was discouraged, BNL was trying to phase them out



From BNL-8381 (1966)

This is an IBM 80 column punchcard



https://en.wikipedia.org/wiki/Punched_card#/media/File:Blue-punch-card-front-horiz.png

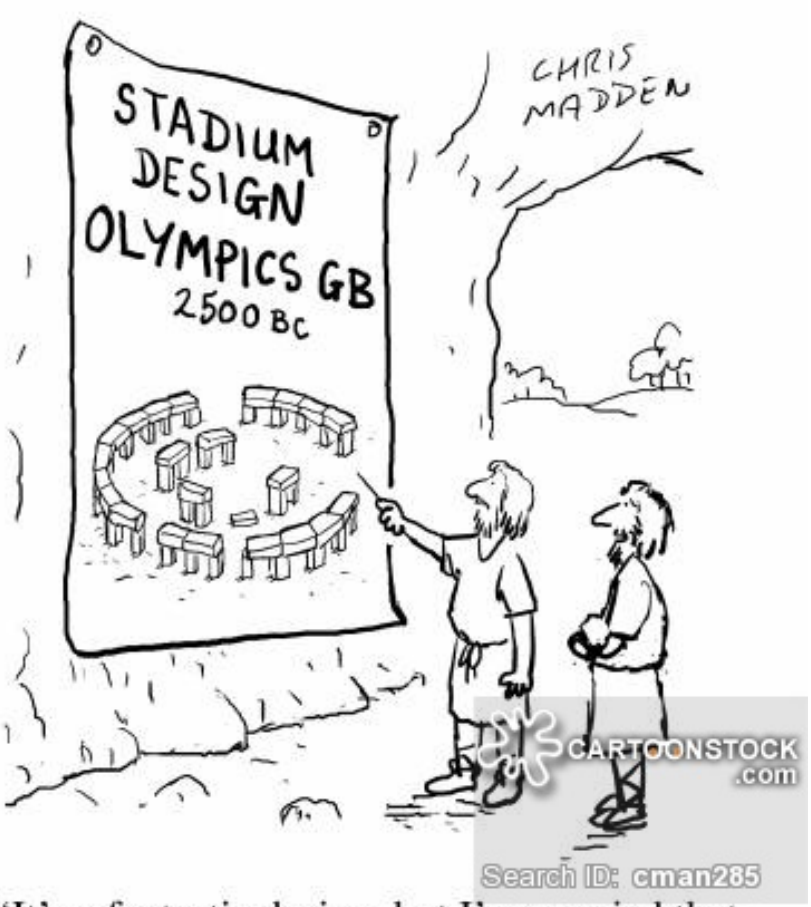
This is a chunk of the n+59Co evaluation: it's punchcard-ready

```
                                  14          83           1          02725 1451   286
                                  14          84           1          02725 1451   287
                                  14          85           1          02725 1451   288
                                  14          86           1          02725 1451   289
                                  14          87           1          02725 1451   290
                                  14          88           1          02725 1451   291
                                                                      2725 1   099999
                                                                      2725 0   0      0
 2.705900+4 5.842690+1            0           0           1          02725 2151     1
 2.705900+4 1.000000+0            0           0           1          02725 2151
 1.000000-5 1.000000+5            1           3           0          12725 2151     3
 3.500000+0 6.672000-1            0           0           2          32725 2151     4
 5.842690+1 6.672000-1            0           0         600        1002725
-5.000000+3 3.000000+0 5.576800+2 9.215100+0 0.000000+0 0.000000+02725
-5.000000+3 4.000000+0 1.898100+2 1.868200-1 0.000000+0 0.000000+02725
-4.767000+2 4.000000+0 1.949000-2 2.148900+0 0.000000+0 0.000000+02725
-2.258800+2 3.000000+0 9.164400+0 5.214100-2 0.000000+0 0.000000+02725
 1.320000+2 4.000000+0 5.270100+0 4.700000-1 0.000000+0 0.000000+02725
 4.323100+3 4.000000+0 1.041400+2 4.173700-1 0.000000+0 0.000000+02725
 5.016000+3 3.000000+0 6.789601+2 1.332200+0 0.000000+0 0.000000+02725
 6.389700+3 4.000000+0 1.681100+0 3.155600-1 0.000000+0 0.000000+02725
```

Line number, so you can put your punchcards back in order if you drop them

ENDF is resilient

- Colony Restaurant closed 1963
- AEC created CSEWG and ENDF; AEC ended in 1974, replaced with DOE in 1977
- ENDF/B-V made “classified”, then unclassified
- Management of CSEWG by DOE “faded away” in the 1990’s, but we kept going
- Internet revolution(s)
- 10 US Gov’t administrations, so far
- 50th (-ish) anniversary this year

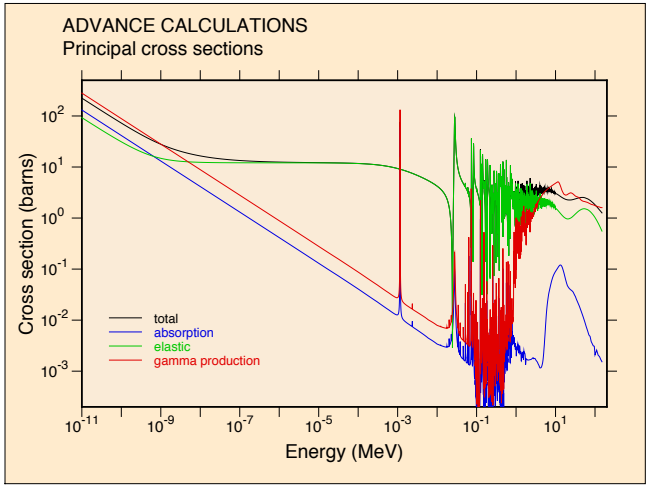


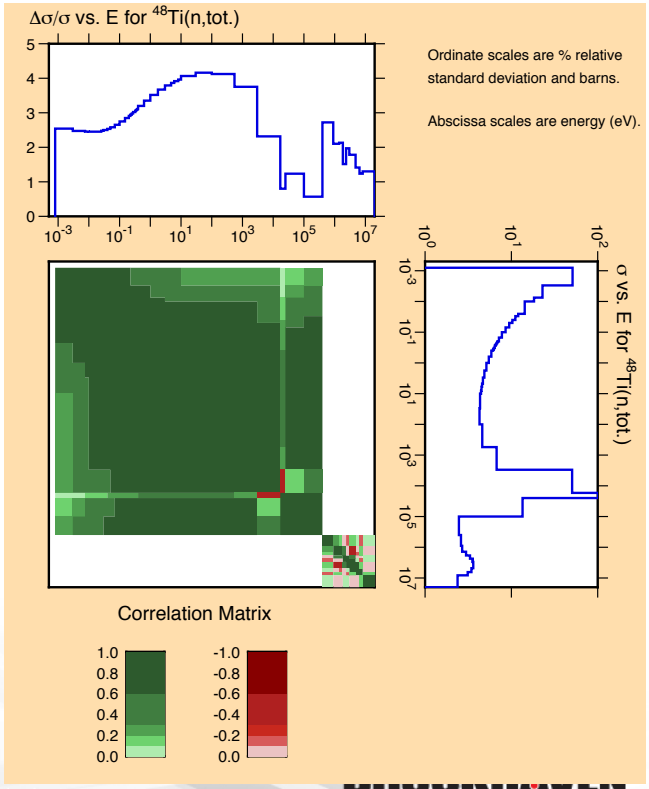
“It’s a fantastic design, but I’m worried that after the games it’ll just end up as a useless load of stone with no legacy potential.”

The most important part of ENDF is the ecosystem built on the format

- PREPRO
- NJOY
- NNDC checking codes
- AMPX
- CALENDF
- …

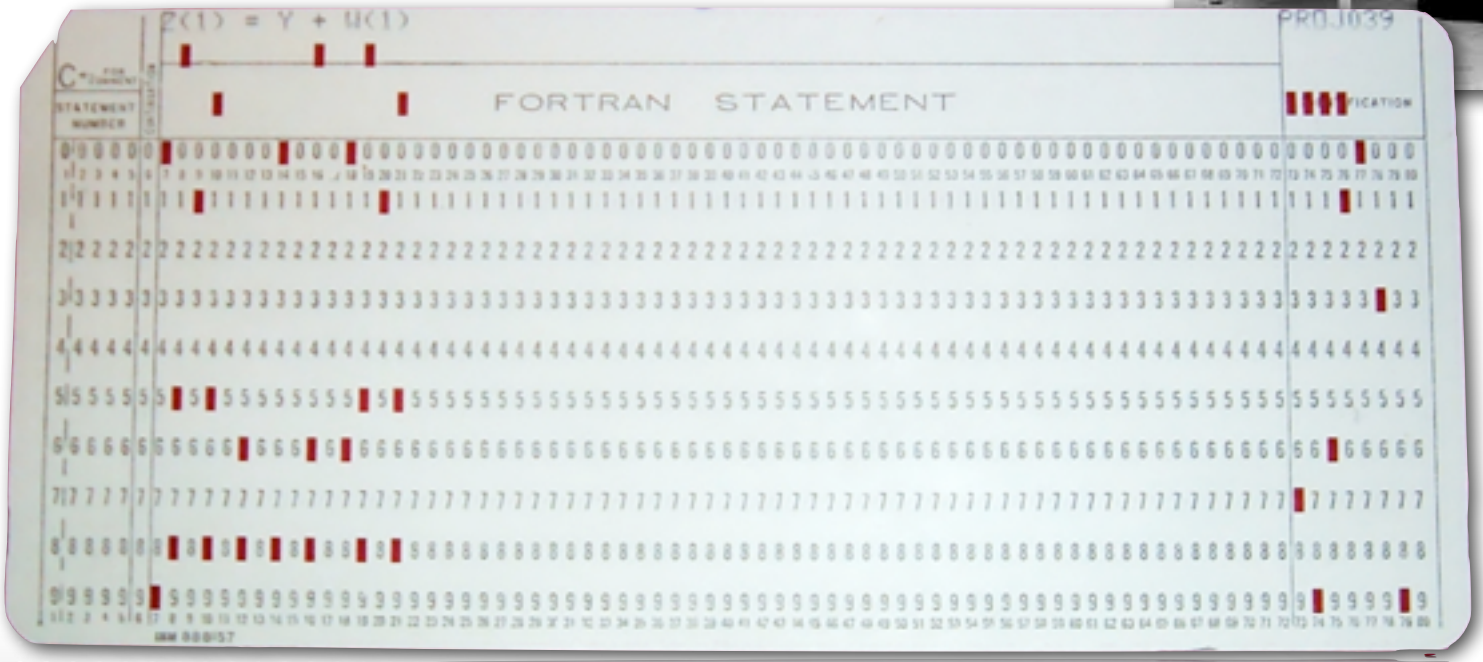
These are the tools that get the data into user's hands





Legacy formats

…but will we continue to be enslaved by this “modern technology”?



No, seriously

- A good format can determine the data structures used to interact with it
- These data structures are the components we use to create new things
- **We are trying to create a development environment (tools + components) that we enjoy working with**
- We will be working with these tools for a long time

Good tools == Happy developers

ENDF is resilient, but…

- **Obsolete (and therefore confusing) constructs**
  - FEND, MEND, SEND and TEND “cards”
  - line numbers (for the punchcards)
- **Limitations imposed by original physical format**
  - Fixed precision
  - Limited MT’s
  - Limited MAT’s
- **“Design by committee”**
  - MF6
  - Fission data in MT1 not MT18
  - Resonances
  - …
- **“Not fun to work with”, is often is barrier for newcomers**

The biggest danger are the legacy tools becoming “black boxes”

- **Original developers are deceased, retired or soon to retire**
  - NJOY (LANL)
    - McFarlane retired
    - Kahler retiring in June
  - PREPRO (IAEA)
    - Cullen retired
  - ndfgen/mcfgen (LLNL)
    - Perkins deceased
  - AMPX (ORNL)
    - Greene retired
  - CALENDF (CEA)
    - Ribon retired
  - NNDC codes (BNL)
    - Dunford deceased
- **“if it ain’t broke, don’t fix it”, but…**

A chance at a do-over

- **Want to preserve the evaluators' intent; but bad format meant evaluators put things in places they don't belong**
  - pseudo levels in 6,7Li (ab)used in MF4, before MF6 developed
  - fission in W
  - "battle over MT's" for high energy reactions
  - gammas in MT3 or 4 rather than with the reaction that produced them
  - …
- **Bad design leads to mistakes, want to engineer them away**
  - Backgrounds in resonance region
  - Multiple ways to store the same thing (gammas in MF12,13,14 vs. gammas in MF6), possible double counting
  - Synchronization issues (masses, levels, …)
  - …

Outline

- History
- The GNDS Project
- Code support and API
- Format Overview
- Current status: GNDS-1.9 vs. 1.10

FUDGE & GND history: an opportunity

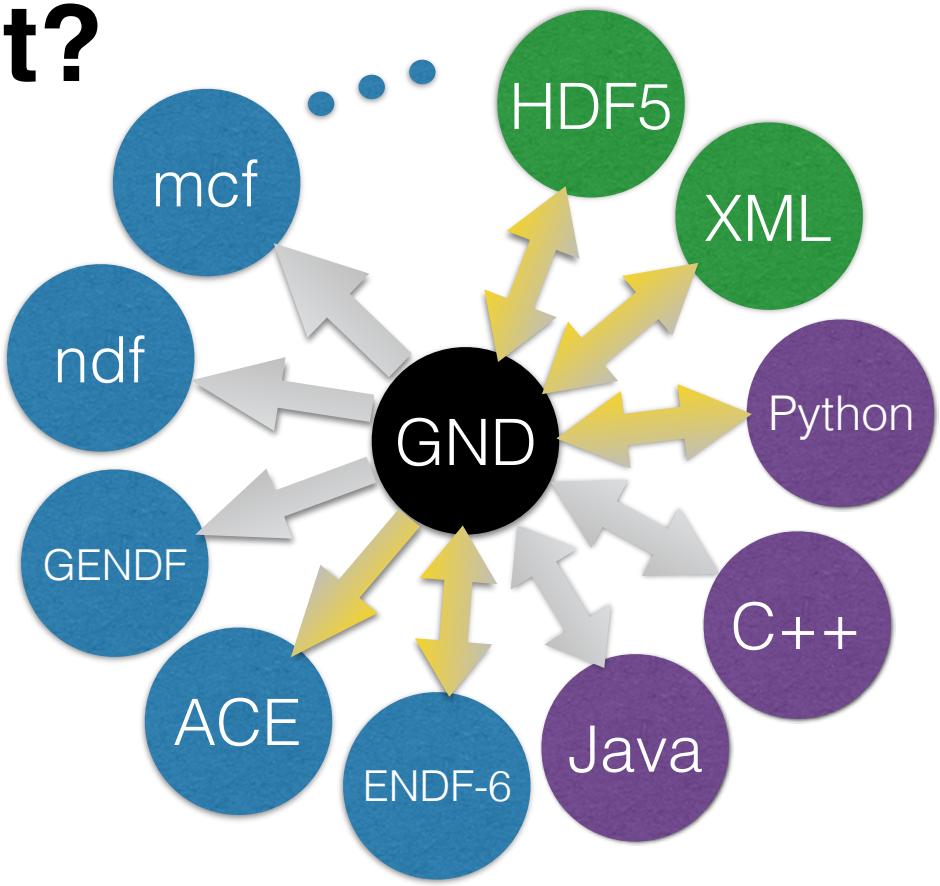
- **LLNL wanted to replace ENDL format (starting ~2005)**
  - Decided against ENDF-6 and for a new structure: GND
  - ARRA funding made it possible
- **Common re-design of format proposed to U.S. CSEWG (2011)**
  - BNL/LANL/ORNL
- **Common re-design of format proposed to NEA-WPEC**
  - SG38 (2012-2016)
  - Focus on redesigning structure and infrastructure
- **Work will continue in SG-43 (2017-2020) and EG-GNDS**

Lawrence Livermore National Laboratory

RECOVERY.GOV

NEA Nuclear Energy Agency

What do (did?) we want to get out of the new format?



- **Both human and computer readable**
  - A textual representation → XML
  - A binary representation → HDF5
- **Extensible**
  - Adding a "new" section should not break any reading code
- **Handle legacy data**
  - Read & possibly correct data
  - Maintain high quality of libraries
- **Make provisions for both evaluated and processed data**
  - Support multiple representations simultaneously (and their dependence)
  - Ex. Resonance parameters and reconstructed pointwise cross sections (0K) and heated cross sections etc.

The work was divided into several WPEC sub-groups

1. **Top-level hierarchy for storing nuclear reaction data**
2. **Hierarchy for storing particle/nucleus data**
3. **Low-level data containers**
4. **API for reading and writing data in the new structure**
5. **Infrastructure for data handling, processing, plotting, etc.**
6. **Defining the tests that will be needed to assure quality of data**
7. **Governance**

SG-38
"Mostly done"
coordinator:
D. McNabb (LLNL)

SG-43
2017-2020
coordinators:
J. Conlin (LANL),
C. Mattoon (LLNL)

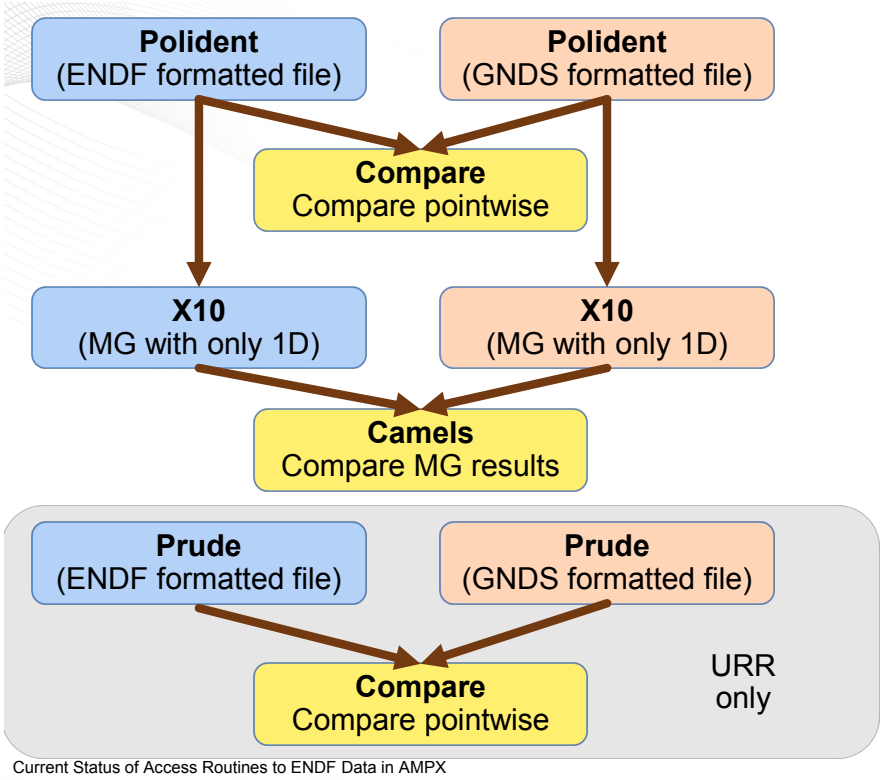
EG-GNDS
chair: D. Brown (BNL)

Outline

- History
- The GNDS Project
- Code support and API
- Format Overview
- Current status: GNDS-1.9 vs. 1.10

Status of GNDS support in processing codes

- **FUDGE (LLNL)** — full support of GNDS-1.9, is reference implementation
- **AMPX (ORNL)** — covariance, resonances supported, partial support of main transport hierarchy
- **NJOY21 (LANL)** —planned, work not yet begun
- **NJOY2016 (LANL)** — will not get GNDS support
- **FRENDY (JAEA)** — not planned at this time
- **GALILEE (CEA)** — planned, work not yet begun



Current Status of Access Routines to ENDF Data in AMPX

AMPX support enabling cross-checks, is finding bugs & improvements in FUDGE

LLNL has 3.5 GNDS APIs

- **PoPs** — properties of particles C++ API
- **GIDI** — I/O classes & routines for transport, C++
- **MCGIDI** — extensions to GIDI for MC transport
- **HAPI** — low level I/O API, include HDF5

WPEC/SG-43 working on more general framework, coordinated by
J. Conlin (LANL) & C. Mattoon (LLNL)

GNDS is in production now

Mercury
GIDI/MCGIDI version 3

Ardra (Sn)
GIDI/MCGIDI version 3

GIDI
MCGIDI
C++
Open source

- **Data QA in ADVANCE**
  - Plotting
  - Rigorous tests
  - Since ENDF/B-VII. 1 (2011)
- **Data Visualization on NNDC and IAEA websites**

GEANT4
A SIMULATION TOOLKIT

G4LND collision kernel
GIDI/MCGIDI version2
Written in C

Slide from M.-A. Descalle
slide based on slide from D. Brown

Testing ENDF/B libraries in GNDS format

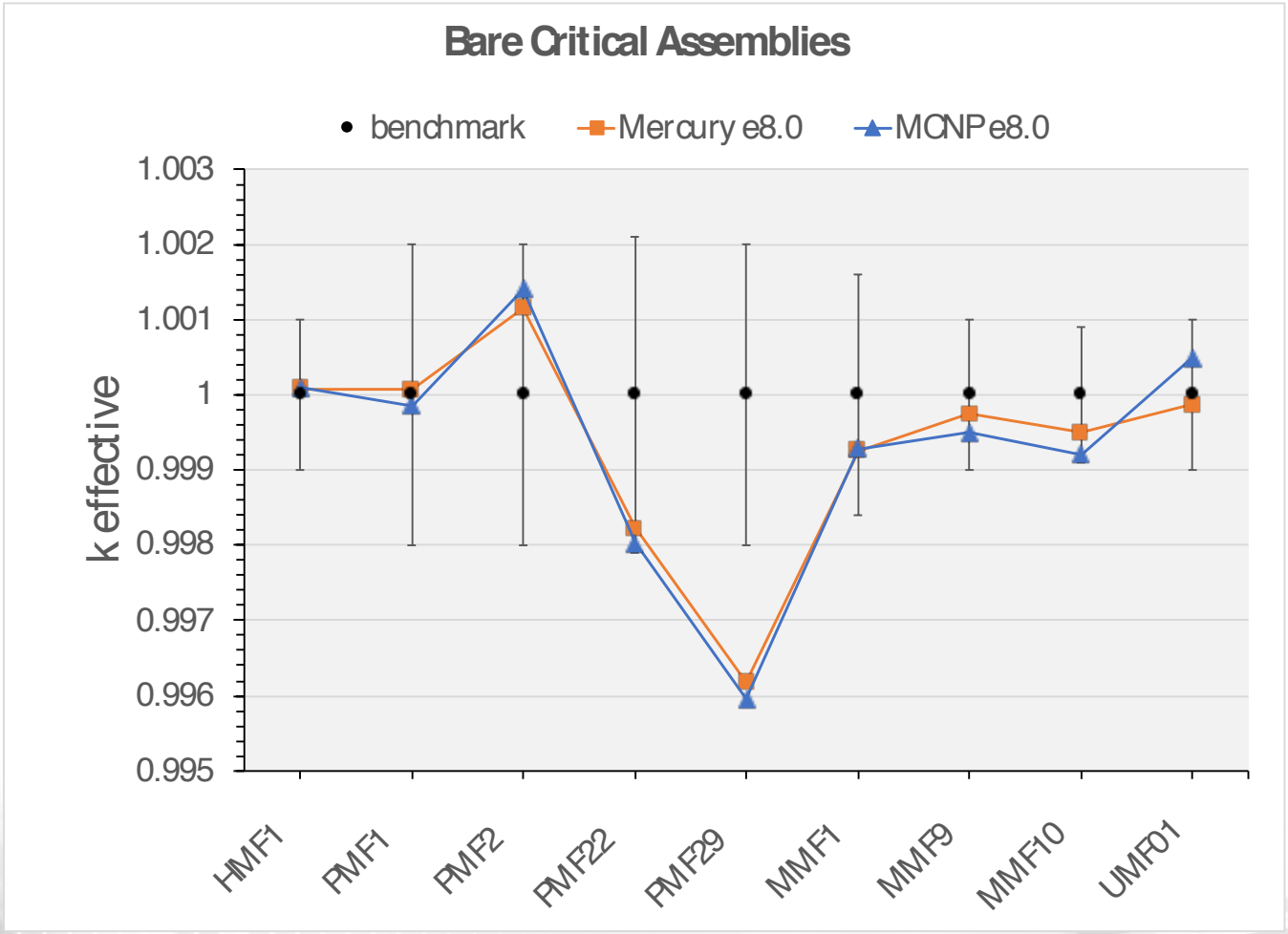
- Two ENDF libraries were translated and processed with FUDGE into GNDS format
  - ENDF/B-VII.1
  - ENDF/B-VIII.0

Code	Code Type	Run mode	Data Format/ API	Benchmark tests	Cross-sections
Mercury	Monte Carlo	Batch	GNDS/ GIDI/ MCGIDI	Criticality: 123 fast assemblies Reaction ratios: 3 assemblies	Continuous Energy
Ardra	Deterministic Sn	Interactive	GNDS/ GIDI	Criticality:79 assemblies	Multigroup: 230 groups

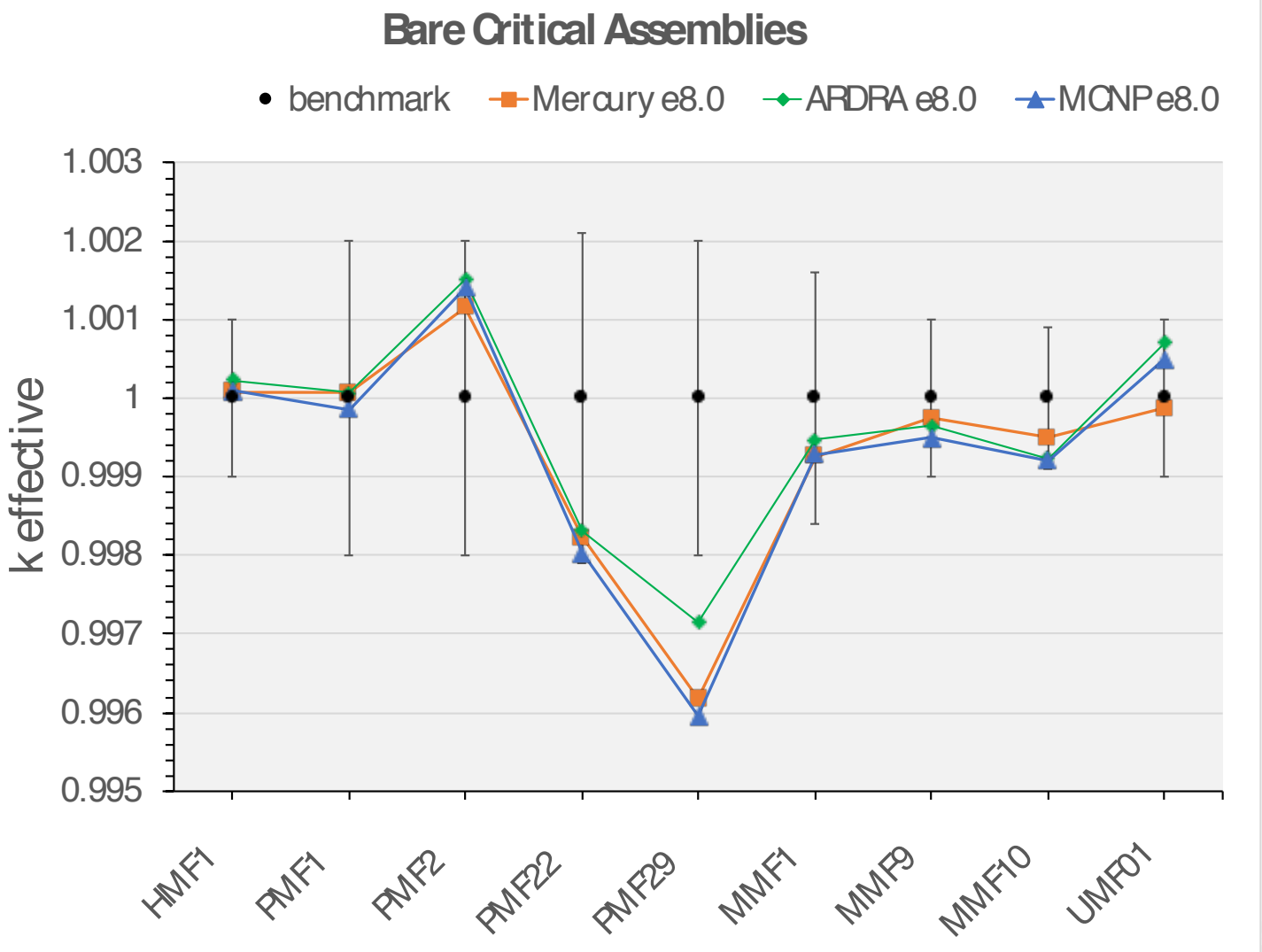
- Results were compared to MCNP6 - ENDF/B-VII.1 and VIII.0 results (2017)

Slide from M.-A. Descalle

Bare assemblies: Godiva, Jezebel, Jezebel240,…



Adding Ardra results



Outline

- History
- The GNDS Project
- Code support and API
- Format Overview
- Current status: GNDS-1.9 vs. 1.10

GNDS is more of an agreed upon hierarchy than a data format

- Can be serialized into any hierarchical data format
  - Currently XML, HDF5
- Well suited to OOP programming paradigm
  - Implementations in Python (FUDGE), C++ (NJOY21, AMPX in progress)
- Hierarchy reflects a mental model well suited to transport codes

GNDS is more of an agreed upon hierarchy than a data format

- Can be serialized into any hierarchical data format
  - Currently XML, HDF5
- Well suited to OOP programming paradigm
  - Implementations in Python (FUDGE), C++ (NJOY21, AMPX in progress)
- Hierarchy reflects a mental model well suited to transport codes

But, data files are boring!

Outline

- History
- The GNDS Project
- Code support and API
- Format Overview
- Current status: GNDS-1.9 vs. 1.10

Plan for completing specifications
Target date is WPEC meeting, May 2019
This will be GNDS-2.0

- **"Freeze" GNDS at GNDS-1.9 with only modest changes between now and the May 2019 WPEC meeting.**
- **ACTION: Complete the requirements documents, ASAP**
- **ACTION: Complete the following extensions/corrections**
  - Corrections to resonances per D. Wiarda EG-GNDS talk
  - Corrections to covariances per D. Wiarda EG-GNDS talk
  - Consistency corrections in TSL data per D. Brown SG-42 talk (<styles> addition, correct <reactionSuite> layering, use of <XYs1d>)
- **ACTION: By Summer 2018, the following format extensions/ corrections will be made or abandoned:**
  - Iterate with A. Sonzogni & J.-C. Sublet the proposed FPY format from B. Beck.
- **ACTION: All changes to GNDS must be complete by June 21, 2018 so that the specifications documents can be updated by September 30, 2018.**
- **ACTION: Review release candidate GNDS-2.0 format at the November CSEWG meeting at BNL, with a teleconferencing option for CNDC, JAEA, CEA and NEA collaborators.**

Plan for completing specifications
Target date is WPEC meeting, May 2019
This will be GNDS-2.0

- **"Freeze" GNDS at GNDS-1.9 with only modest changes between now and the May 2019 WPEC meeting.**
- **ACTION: Complete the requirements documents, ASAP**
- **ACTION: Complete [illegible] extensions/correcti[illegible]**
  - Corrections to resonances per D. Wiarda EG-GNDS talk
  - Corrections to covariances per D. Wiarda EG-GNDS talk
  - Consistency corrections in TSL data per D. Brown SG-42 talk (<styles> addition, correct <reactionSuite> layering, use of <XYs1d>)

We are way behind

- **ACTION: By Summer 2018, the following format extensions/ corrections will be made or abandoned:**
  - Iterate with A. Sonzogni & J.-C. Sublet the proposed FPY format [illegible]eck.
- **[illegible]hanges to GNDS must be complete by June 21, 2018 so that the specifications documents can be updated by September 30, 2018.**
- **ACTION: Review release candidate GNDS-2.0 format at the November CSEWG meeting at BNL, with a teleconferencing option for CNDC, JAEA, CEA and NEA collaborators.**

Multiple sources of formatting information, all different, none complete and some out of date

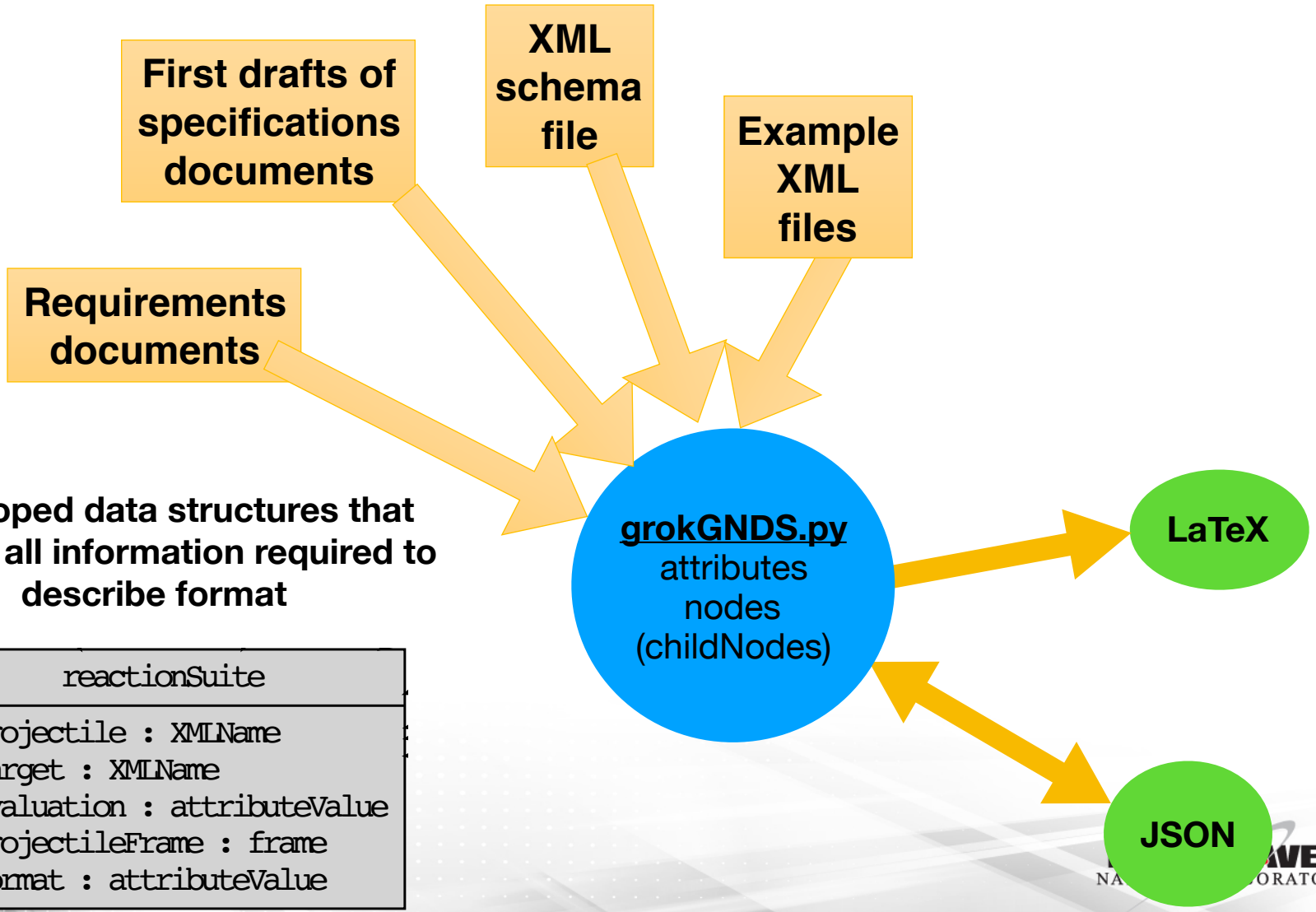
First drafts of specifications documents

XML schema file

Example XML files

Requirements documents

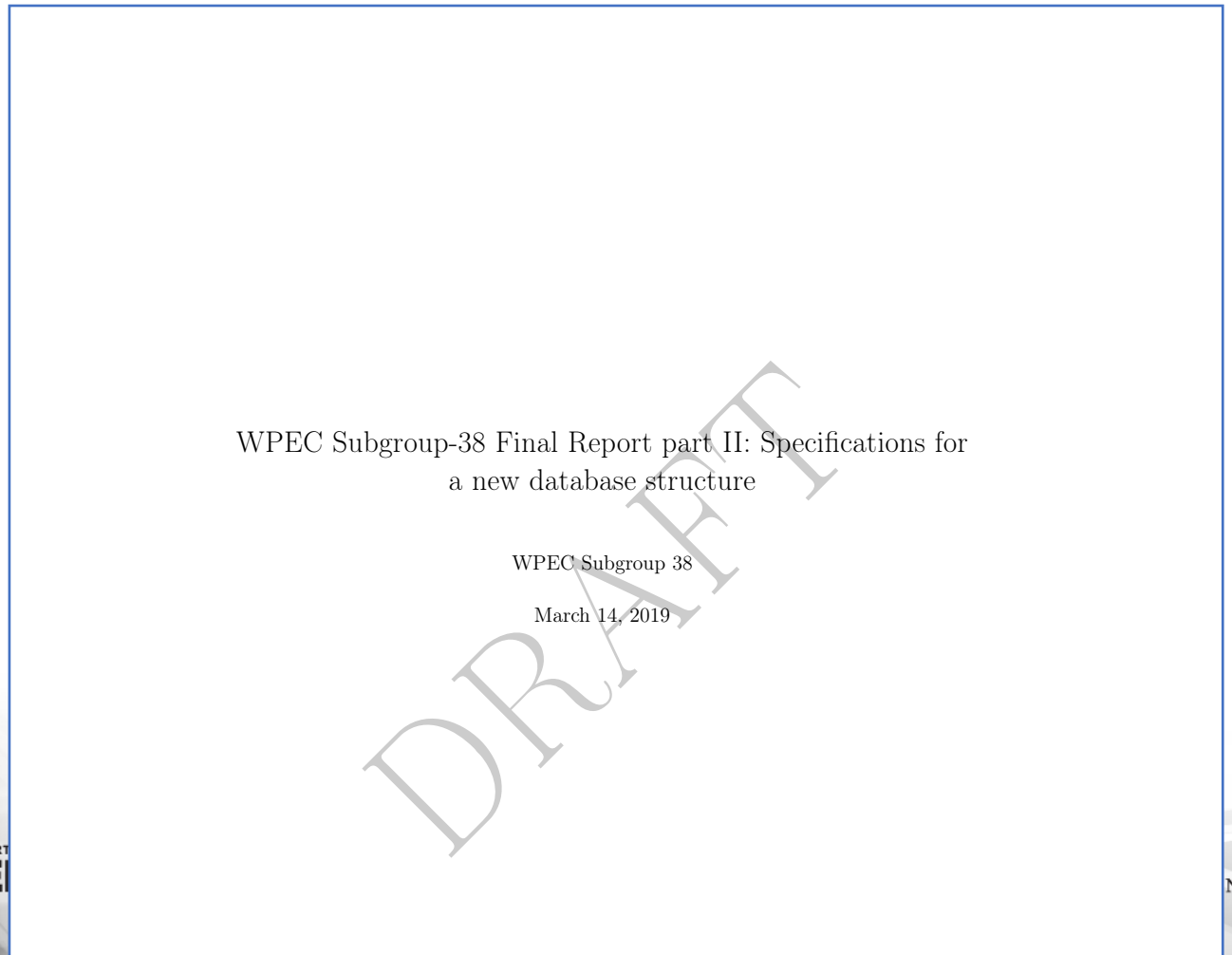
Multiple sources of formatting information, all different, none complete and some out of date



Developed data structures that contain all information required to describe format

reactionSuite
+ projectile : XMLName + target : XMLName + evaluation : attributeValue + projectileFrame : frame + format : attributeValue

Draft specifications for GNDS-1.9 are under active development


WPEC Subgroup-38 Final Report part II: Specifications for a new database structure

WPEC Subgroup 38

March 14, 2019

DRAFT

There's still a lot to do and problem areas remain

- **Corrections in resonances formats** (e.g. <spin> used differently in RRR and particle specifications)
- **Corrections in covariance formats**
- **Inconsistencies uncovered during tree-walking of existing files & schema**
- **GNDS-1.9 TSL data:** quick translation of ENDF-6, modest revisions to make it consistent with rest of transport data
- **GNDS-1.9 FPY data:** quick translation of ENDF-6, significant changes needed to satisfy users & requirements

GNDS-1.10 is contains TSL, FPY formats from LLNL

ENDF library status

- Next major release of ENDF to be released in both GNDS and ENDF-6 formats
  - ENDF/B-VIII.1 already released in GNDS-1.9
- Plan for JEFF-4 to be released in both formats
- Currently JENDL taking a “wait and see” approach